

# Crystal structures of Hydrogen and Deuterium Iodide

## HI and DI

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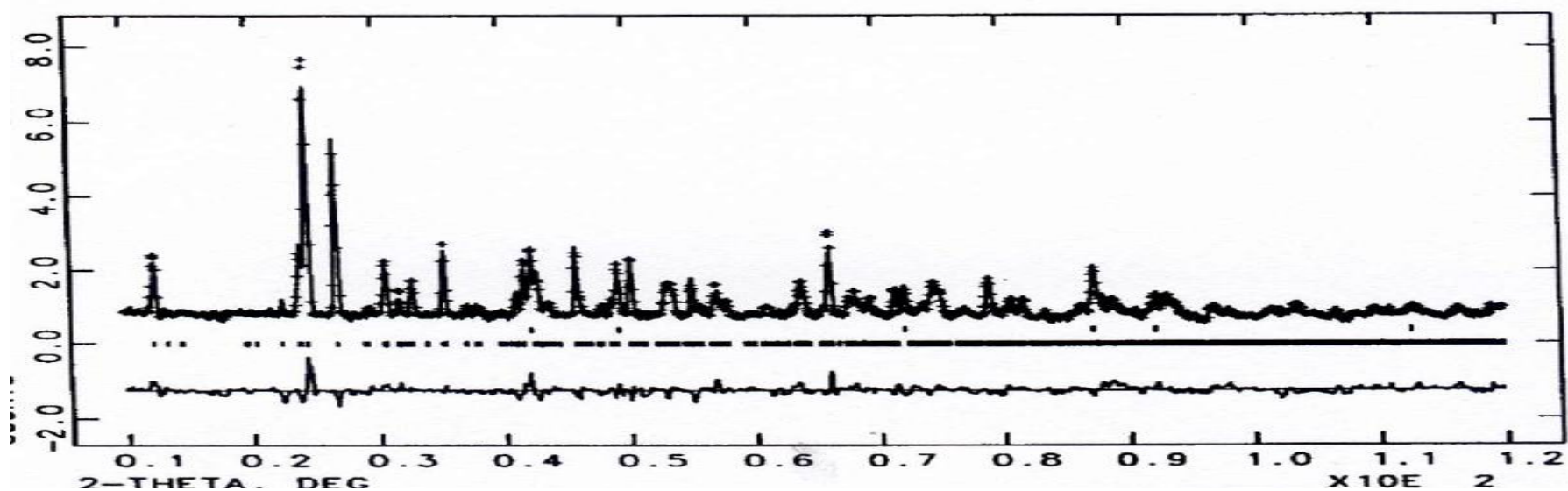
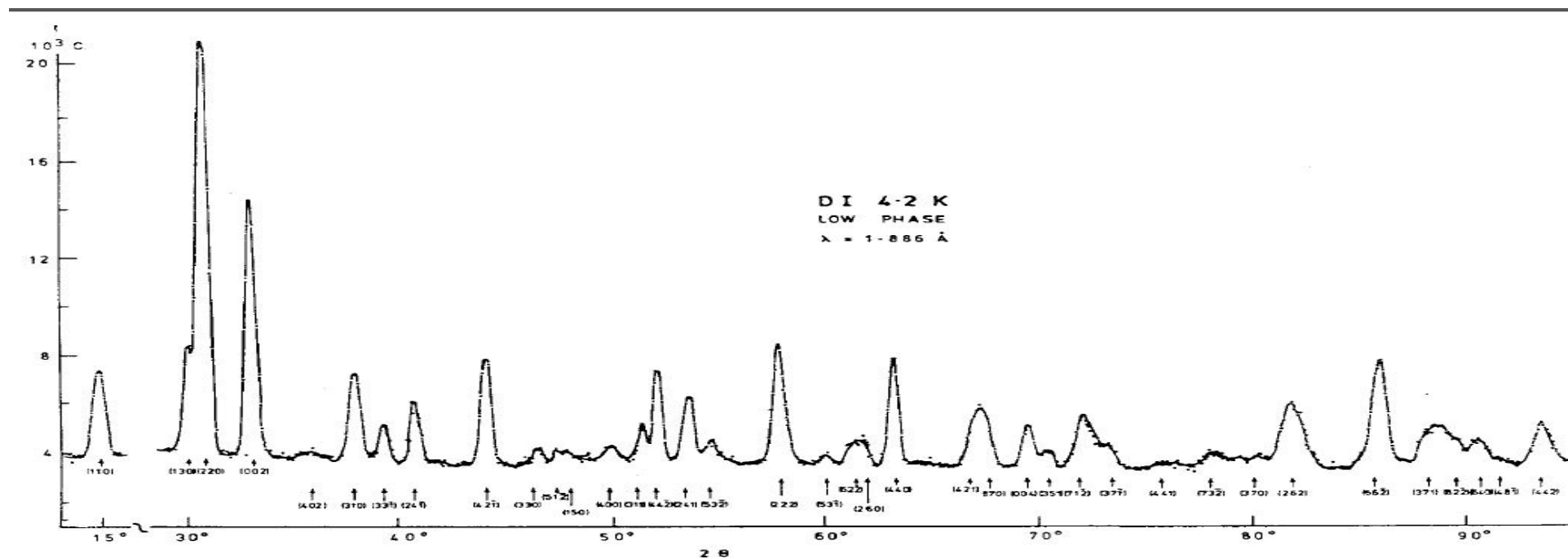
The incomplete determination of the low phase structure of DI in my thesis of 1971 was a source of regret. The 1993 paper by Ikram, Torrie and Powell<sup>i</sup> published the solved version. However, the thesis work which covered the X-ray work and the middle and high phases and the phase transition measurements and hysteresis was never published so was not referenced.

The 1971 thesis was posted on the web some time ago at

<https://archive.org/details/CrystalStructureAndPhaseTransitionsOfSolidDeuteriumIodidePhDThesis>

A simple comparison of the low phase scattering patterns between the Panda run at 1.6 Å and Ikram's pattern look comfortably similar for the first 8 peaks at low theta although the statistics and resolution of Ikram's data are obviously much better.

It is shown as a simple comparison and it satisfies historic concerns about impurities in my sample or preferred orientation. I think when our group leader and supervisor Endre Sandor<sup>ii</sup> suggested we considered a larger monoclinic unit cell it seemed a bold step - in fact it was triclinic with little symmetry. Whether my data were of good enough resolution to have determined the true structure is probably doubtful.



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<sup>ii</sup> <http://ph.qmul.ac.uk/sites/default/files/brochure1963.pdf>